

Bowers  
230355

## FINAL REPORT

March 1, 1996 to August 31, 1999

Cluster Ions  
AFOSR Grant F49620-96-1-0033  
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Santa Barbara, CA 93106

### I. Abstract/Status

Progress has been made on the objectives listed below. The structure and energetics of a number of important synthetic polymers have been successfully investigated. A successful model for the gas phase H/D exchange mechanism for proteins has been developed. Progress has been made on determining the basis for gas phase salt bridge formation in biopolymers. Finally, promising results have been obtained on the reactivity, energetics and structures of transition metal/benzene clusters. At present, we are developing theoretical models to help us interpret the data. Finally, the design of a new instrument has been completed and construction initiated.

### II. Objectives

- A. Characterization of the Gas Phase Growth Mechanisms, Conformations and Energetics of:
- B.
  - 1. Metallic/Molecular clusters and composite materials.
  - 2. Synthetic and biopolymers
  - 3. Host/Guest Pairs
- C. Development of Experimental and theoretical methodology needed for Part A.

### III. Progress/Accomplishments

The progress we have made to date on this grant has been given in great detail in the renewal proposal submitted in April, 1998, as well as in prior progress reports. The work in progress discussed there has been mostly completed as evidenced by the publications listed next.

### IV. Papers Published or Submitted for Publication

#### A. Published

- 1. Mass Spectrometry: Recent Advances and Future Directions, Michael T. Bowers, Alan G. Marshall and Fred W. McLafferty Journal of Physical Chemistry, Centennial Issue, 100, 12897 (1996). (1997).

2. The Gas Phase Conformation of Biological Molecules: Bradykinin, Thomas Wytttenbach, Gert von Helden and Michael T. Bowers, *J. Am. Chem. Soc.* **118**, 8355 (1996).
3. Effect of the Long Range Potential on Ion Mobility Measurements, Thomas Wytttenbach, Gert von Helden, Joseph T. Batka, Jr., Douglas Carlat and Michael T. Bowers, *J. Am. Soc. Mass Spectrom.*, **8**, 275 (1997).
4. Structures of  $C_nH_x^+$  Molecules for  $n \leq 22$  and  $x \leq 5$ : The Emergence of PAHs and the Effects of Dangling Bonds on Conformation, Seonghoon Lee, Nigel Gotts, Gert von Helden and Michael T. Bowers *J. Phys. Chem. A*, **101**, 2096 (1997).
5. Gas Phase Structures of Sodiated Oligosaccharides by Ion Mobility/Ion Chromatography Methods, Seonghoon Lee, Thomas Wytttenbach and Michael T. Bowers, *Int. J. Mass Spectrom. Ion Proc. Chava Lifshitz Honor Issue*, **167/168**, 605 (1997).
6. Structures and Energetics of  $V_n(C_6H_6)_m^+$  Clusters: Evidence for a Quintuple Decker Sandwich, Patrick Weis, Paul R. Kemper and Michael T. Bowers, *J. Phys. Chem. A*, **101**, 8207 (1997).
7. Conformations of Alkali Ion Cationized Polyethers in the Gas Phase: poly[ethylene glycol] and bis [(benzo-15-crown-5)-15-ylmethyl] pimelate, *Int. J. Mass Spectrom. Ion Proc. Keith Jennings Honor Issue*, **165/166**, 377 (1997).
8. The Effect of the Variation of Cation in the Matrix-Assisted Laser Desorption/Ionization-Collision Induced Dissociation (MALDI-CID) Spectra of Oligomeric Systems, James H. Scrivens, Anthony T. Jackson, Hilary T. Yates, Martin R. Green, Glen Critchley, Jeff Brown, Robert H. Bateman, Michael T. Bowers and Jennifer Gidden, *Int. J. Mass Spectrom. Ion Proc. Keith Jennings Honor Issue*, **165/166**, 365 (1997).
9. Salt Bridge Structures in the Absence of Solvent? The Case for the Oligoglycines, Thomas Wytttenbach, John E. Bushnell and Michael T. Bowers, *J. Am. Chem. Soc.*, **120**, 5098-5103 (1998).
10. Cluster Assisted Thermal Energy Activation of the H-H Sigma Bond in  $H_2$  by Ground State  $B^+(^1S_1)$  Ions: Overcoming a 77 kcal/mol Barrier, Paul R. Kemper, John E. Bushnell, Patrick Weis and Michael T. Bowers, *J. Am. Chem. Soc.*, **120**, 7577 (1998).
11. Binding Between Ground State Aluminum Ions and Small Molecules:  $Al^+(H_2/CH_4/C_2H_2/C_2H_4/C_2H_6)_n$ ; Can  $Al^+$  Insert into  $H_2$ ?, Paul R. Kemper, John E. Bushnell, Michael T. Bowers and Greg I. Gellene, *J. Phys. Chem.*, Sidney Benson Honor Issue, **102**, 8590 (1998).

12. Gas Phase Conformations of Biological Molecules: The Hydrogen/Deuterium Exchange Mechanism, Thomas Wyttenbach and Michael T. Bowers, *J. Am. Soc. Mass Spectrom.*, **10**, 9 (1999)
13. Gas Phase Conformations of Synthetic Polymers: Poly (Methyl Methacrylate) (PMMA) Oligomers Cationized by Sodium Ions, Jennifer Gidden, Anthony T. Jackson, James H. Scrivens and Michael T. Bowers, *Int. J. Mass Spectrom.*, Brian Green Honor Issue, **188**, 121 (1999)
14. Folding Energetics and Dynamics of Macromolecules in the Gas Phase: Alkali Ion Cationized Poly (Ethylene Terephthalate) (PET) Oligomers, Jennifer Gidden, Thomas Wyttenbach, Joseph J. Batka, Patrick Weis, Anthony T. Jackson, James H. Scrivens and M.T. Bowers, *J. Am. Chem. Soc.*, **121**, 1421 (1999).
15. Energetics and Structures of Gas Phase Ions: Macromolecules, Clusters and Ligated Transition Metals, Michael T. Bowers, Paul R. Kemper, Petra van Koppen, Thomas Wyttenbach, Catherine J. Carpenter, Patrick Weis and Jennifer Gidden, NATO ASI, "Energetics of Stable Molecules and Reactive Intermediates," Castelo Branco, Portugal, July, 1998, pp. 235-258.
16. Poly (ethylene terphthalate) (PET) Oligomers Cationized by Alkali Ions: Structures, Energetics and Their Effects on Mass Spectra and the MALDI Process, Jennifer Gidden, Thomas Wyttenbach, Joseph J. Batka, Patrick Weis, Anthony T. Jackson, James H. Scrivens, and Michael T. Bowers, *J. Am. Soc. Mass Spectrom.*, R. Squires Beimann Medal Special Issue **10/9** 883 (1999)

## V. Personnel Supported

### A. Senior

Dr. Paul Kemper  
 Dr. Seunghoon Lee  
 Dr. Joseph Batka  
 Dr. Thomas Wyttenbach  
 Dr. Patrick Weis

### B. Junior

Ms. Jennifer Gidden  
 Mr. Travis Walkup  
 Mr. Peter Nishamura

## **VI. Papers Presented**

### **A. Invited Lectures at Meetings**

1. Field and Franklin Award Address, Award Symposium, Analytical Division, American Chemical Society, New Orleans, LA, March 1996.
2. Invited Lecturer, Gordon Conference on Molecular and Ionic Clusters, Barga, Italy, May 1996.
3. Keynote Lecturer, Symposium on the Structure and Energetics of Ions, American Society of Mass Spectrometry, Portland, OR, May 1996.
4. Invited Speaker, Air Force Contractors Meeting, Boulder, CO, July 1996.
5. Invited Speaker, Eighth International Symposium on Small Particles and Inorganic Clusters, Copenhagen, Denmark, July 1996.
6. Invited Lecturer, Gordon Conference on the Structure, Dynamics and Energetics of Gaseous Ions, Ventura, CA, February 1997.
7. Plenary Lecture, New Methods in Ion Cyclotron Resonance, Tallahassee, FL, March 1997.
8. Invited Speaker, Biological Applications of Mass Spectrometry, Pittsburg Conference, Atlanta, GA, March 1997.
9. Invited Speaker, Symposium on Polyethylene Glycol, American Chemical Society Meeting, San Francisco, CA, April 1997.
10. Invited Speaker, Fisher Award Symposium, American Chemical Society Meeting, San Francisco, CA, April 1997.
11. Invited Speaker, International Congress of Quantum Chemistry, Atlanta, GA, June 1997.
12. Plenary Lecture, Portuguese Mass Spectrometry Society, Lisbon, Portugal, September 1997
13. Invited Speaker, Symposium on Mass Spectrometry, Pacific Conference on Chemistry and Spectroscopy, Irvine, CA, October 1997.
14. Invited Speaker and Organizer, The Jennings Symposium, Warwick University, United Kingdom, December 1997.
15. Invited Speaker and Organizer, Field and Franklin Award Symposium, American Chemical Society Meeting, Dallas, TX, April 1998.

16. Invited Lecturer, AFOSR Contractors Meeting, Monterey, CA, May 1998
17. Invited Speaker and Organizer, Ion Structure and Energetics Symposium, American Society for Mass Spectrometry, Orlando FL, June 1998
18. Invited Speaker (2 lectures) NATO Advanced Study Institute "Energetics of Stable Molecules and Reactive Intermediates," Castelo Branco, Portugal, July 1998
19. Invited Speaker, Tutorial Lecture on "The Anatomy of a Collision and Its Consequences," 47th National Meeting, American Society for Mass Spectrometry, Dallas, TX, May, 1999

#### **B. Contributed Papers**

1. Presented 5 oral papers, West Coast Ion Chemistry Conference, Lake Arrowhead, CA, January 1997.
2. Presented 2 posters, Gordon Conference on the Structure, Dynamics and Energetics of Gaseous Ions, Ventura, CA, February 1997.
3. Presented 3 oral papers and 3 posters, American Society for Mass Spectrometry Conference, Palm Springs, CA, June 1997.
4. Presented 4 oral papers, West Coast Ion Chemistry Conference, Lake Arrowhead, CA, January 1998
5. Presented 2 oral papers, American Society of Mass Spectrometry, Orlando, FL, June 1998
6. Presented 4 oral papers, West Coast Ion Chemistry conference, Lake Arrowhead, CA, January 1999
7. Presented oral paper, Symposium on Industrial Polymers, 47th Annual American Society of Mass Spectrometry Meeting, Dallas, TX, May 1999

#### **C. Seminars**

1. University of Chicago, February 1996.
2. University of Warwick (UK), December 1996.
3. Purdue University, January 1997.
4. Colorado State University, March 1997.
5. University of Colorado, Boulder, March 1997.

6. Michigan State University, March 1997.
7. Northwestern University, March 1997.
8. University of Washington, May 1997.
9. Pacific Northwest National Lab, May 1997.
10. Prims Lecturer, Syracuse University, Syracuse, NY, October 1997.
11. Cornell University, Ithica, NY, October 1997.
12. Bircher Lecturer, Vanderbilt University, Nashville, TN, November 1997
13. Gonzaga University, Spokane, WN, November, 1997
14. University of Nevada at Reno, Reno, Nevada, March 1998
15. California Institute of Technology, Pasadena, CA, April 1999
16. Westmont College, Santa Barbara, CA, April 1999

## **VII. Honors and Awards**

### **A. Current**

Special issue published in my honor, International Journal of Mass Spectrometry, Vols. 185, 186, 187, June (1999)

### **B. Continuing/Prior**

1. Fellow, American Physical Society (elected 1987)
2. Fellow, American Association of the Advancement of Science (elected 1994).
3. Fellow, John Simon Guggenheim Foundation (1995 calendar year).
4. Nobel Laureate Signature Award, American Chemical Society (1989).
5. Faculty Research Lecturer, University of California at Santa Barbara (1994).
6. Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry, American Chemical Society, March 1996.
7. The Thomson Gold Medal (1997). This medal is the highest honor awarded internationally in Mass Spectrometry.

### **VIII. Transitions**

Work continues in collaboration with the group at ICI Ltd. Details are given in prior reports.

### **IX. New Discoveries, Inventions or Patent Disclosures**

None

## REPORT DOCUMENTATION PAGE

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## 13. ABSTRACT (Maximum 200 words)

Progress has been made on the objectives listed below. The structures and energetics of a number of important synthetic polymers have been successfully investigated. A successful model for the gas phase H/D exchange mechanism for proteins has been developed. Progress has been made on determining the basis for gas phase salt bridge formation in biopolymers. Finally, promising results have been obtained on the reactivity, energetics and structures of transition metal/benzene clusters. At present, we are developing theoretical models to help us interpret the data. Finally, the design of a new instrument has been completed and construction initiated.

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